(FILE 'HOME' ENTERED AT 18:01:32 ON 04 APR 2004) FILE 'REGISTRY' ENTERED AT 18:01:37 ON 04 APR 2004 L1STRUCTURE UPLOADED L20 S L1 FULL L3STRUCTURE UPLOADED L42 S L3 FULL FILE 'CAPLUS' ENTERED AT 18:03:17 ON 04 APR 2004 L5 3 S L4 FILE 'REGISTRY' ENTERED AT 18:03:55 ON 04 APR 2004 L6 STRUCTURE UPLOADED 0 S L6 FULL L7 =>

```
C:\Program Files\Stnexp\Queries\800c.str
                                                                                     e 7
chain nodes :
```

```
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 27 28 34 35 36 37 38 39 40 41 42 43 44 45 46 47 57 60 61
ring nodes :
      29 30
                 31 32 33
chain bonds
      1-2 1-28 1-60 2-3 3-4 4-27 5-6 6-7 7-8 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17 17-61 18-19 18-61 19-20 20-21 21-22 22-23 33-57 34-35 36-40 37-41
      15-16 16-17
                39-43 44-46 45-47
      38-42
ring bonds :
      29-30 29-33 30-31 31-32 32-33
exact/norm bonds :
                                   4-27 29-30 29-33 30-31 31-32 32-33 33-57
      1-2 1-60 2-3 3-4
exact bonds :
     1-28 5-6 6-7 7-8 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17 17-61 18-19 18-61 19-20 20-21 21-22 22-23 34-35 36-40 37-41 38-42 39-43 44-46 45-47
G1: [*1], [*2]
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ph,[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9]
G3:[*11]
Match level:
     1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
     35:Atom 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 57:CLASS 60:CLASS 61:CLASS
```

```
C:\Program Files\Stnexp\Queries\800c.str
                                                                                                   e 39-----43
chain nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 27 28 34 35 36 37 38 39 40 41 42 43 44 45 46 47 57 60 61
ring nodes :
    29 30 31 32 33
chain bonds
```

```
Chain bonds:
    1-2 1-28 1-60 2-3 3-4 4-27 5-6 6-7 7-8 8-9 9-10 10-11 11-12 13-14 14-15
    15-16 16-17 17-61 18-19 18-61 19-20 20-21 21-22 22-23 33-57 34-35 36-40 37-41
    38-42 39-43 44-46 45-47

ring bonds:
    29-30 29-33 30-31 31-32 32-33

exact/norm bonds:
    1-2 1-60 2-3 3-4 4-27 29-30 29-33 30-31 31-32 32-33 33-57

exact bonds:
    1-28 5-6 6-7 7-8 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17 17-61 18-19
    18-61 19-20 20-21 21-22 22-23 34-35 36-40 37-41 38-42 39-43 44-46 45-47

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ph,[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9]

G3:[*11]

Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS 37:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 57:CLASS 57:CLASS 60:CLASS 61:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 57:CLASS 57:CLASS 60:CLASS 61:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 57:CLASS 57:CLASS 60:CLASS 61:CLASS 57:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 45:CLASS 47:CLASS 57:CLASS 57:CLASS 60:CLASS 61:CLASS 57:CLASS 57:CLASS 57:CLASS 60:CLASS 61:CLASS 57:CLASS 57:CLASS 57:CLASS 57:CLASS 57:CLASS 60:CLASS 61:CLASS 61:CLASS
```

```
C:\Program Files\Stnexp\Queries\800d.str
```

```
1 2 3
                    5 6 7 8 9 10 11 12 13 14 15 16 17
                                                                             18 19 20 21 22 23 27 28
     32 39
ring nodes :
     33 34 35 36 37 38
chain bonds
     1-2 1-28 1-36 2-3 3-4 4-27 5-6 6-7 7-8 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17 17-32 18-19 18-32 19-20 20-21 21-22 22-23 33-39
ring bonds : 33-34 33-38 34-35 35-36 36-37 37-38
exact/norm bonds :
     1-2 2-3 3-4 4-27
exact bonds:
     1-28 1-36 5-6 6-7 7-8 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17 17-32
     18-19 18-32 19-20 20-21 21-22 22-23 33-39
normalized bonds:
33-34 33-38 34-35 35-36 36-37 37-38
G1:[*1],[*2]
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ph,[*1],[*2]
G3
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:Atom 27:Atom 28:Atom 32:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
     38:Atom 39:CLASS
```

chain nodes :